

What is claimed is:

1. A method for mounting a sample comprising a crystal, said method comprising the steps of:
  - 5 (a) providing a crystal holder containing at least one crystal;
  - (b) providing a tool capable of retrieving said crystal holder, said tool movable by means of a robot;
  - (c) providing a positioning device for mounting said crystal holder so that said crystal is in the path of a beam of X-rays; and
  - 10 (d) activating said robot so that said tool retrieves said crystal holder, transfers said retrieved crystal holder to said positioning device, and mounts said transferred crystal holder on said positioning device.
2. The method of claim 1, wherein said crystal holder is mounted to  
15 said positioning device by means of screw threads.
3. The method of claim 1, wherein said crystal in said retrieved crystal holder is shielded from air.
- 20 4. The method of claim 1, wherein said crystal in said retrieved crystal holder is maintained at a temperature not in excess of about 160° K.
5. A method for aligning a sample comprising a crystal, said sample mounted on a positioning device, said method comprising the steps of:
  - 25 (a) providing a sample, said sample mounted on a positioning device;
  - (b) providing an apparatus capable of viewing said mounted sample, whereby said apparatus is capable of imaging said mounted sample and determining coordinates of said sample relative to a reference position;
  - (c) providing a source of power for adjusting said positioning device  
30 linearly along three orthogonal axes and rotationally about one of said three axes; and

(d) activating said source of power to cause said positioning device to be adjusted such that said sample is positioned into the path of a beam of X-rays, said adjustment of said positioning device being at a plurality of angles, such that said sample is positioned within said beam of X-rays at any angle of rotational adjustment.

6. The method of claim 5, wherein said viewing apparatus is a CCD camera.

7. The method of claim 5, wherein said source of power comprises at least one motor.

8. The method of claim 5, wherein said plurality of angles ranges from 0° to 90°.

9. The method of claim 5, wherein said positioning of said sample involves a least squares fit of offset data collected along said three orthogonal axes at said plurality of angles to an equation.

10. The method of claim 9, wherein said equation for two of said three orthogonal axes is

$$V_i = \Delta X \cos \phi_i + \Delta Y \sin \phi_i$$

where  $V_i$  represents the vertical offset of the centroid of the image of said sample at an angle  $\phi_i$ , and  $\Delta X$  represents the unknown offset of the centroid of the image of the sample from the X-axis and  $\Delta Y$  the represents the unknown offset of the centroid of the image of the sample from the Y-axis.

11. The method of claim 10, wherein said equation for said third of said three orthogonal axes employs a simple average of offset data at said plurality of angles.

- 5           12. A method for conducting X-ray scatter analysis on a sample selected from a plurality of samples, said sample containing a crystal, said method comprising the steps of:
- (a) providing a crystal holder containing at least a crystal, said crystal holder contained in a storage cell;
  - 10       (b) providing a tool capable of retrieving said crystal holder, said tool movable by means of a robot;
  - (c) providing a positioning device for mounting said crystal holder so that said crystal is in the path of a beam of X-rays;
  - (d) activating said robot so that said tool retrieves said crystal holder  
15 from said storage cell, transfers said retrieved crystal holder to said positioning device, and mounts said transferred crystal holder on said positioning device;
  - (e) providing an apparatus capable of viewing said mounted sample, whereby said apparatus is capable of imaging said mounted sample and determining coordinates of said sample relative to a reference position;
  - 20       (f) providing a source of power for adjusting said positioning device linearly along three orthogonal axes and rotationally about one of said three axes;
  - (g) activating said source of power to cause said positioning device to be adjusted such that said sample is positioned into the path of a beam of X-  
25 rays, said adjustment of said positioning device being at a plurality of angles, such that said sample is positioned within said beam of X-rays at any angle of rotational adjustment;
  - (h) providing a beam of X-rays, said beam aimed at said sample;
  - (i) recording scattering of X-rays from said sample; and

(j) activating said robot so that said tool retrieves said crystal holder from said positioning device and transfers said crystal holder retrieved from said positioning device to said storage cell.

5           13.    The method of claim 12, wherein said crystal holder is mounted to said positioning device by means of screw threads.

          14.    The method of claim 12, wherein said crystal in said retrieved crystal holder is shielded from air.

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          15.    The method of claim 12, wherein said crystal in said retrieved crystal holder is maintained at a temperature not in excess of about 160° K.

          16.    The method of claim 12, wherein a computer is employed to  
15    automate said method.

          17.    The method of claim 12, wherein a computer is employed to record scattering of X-rays from said sample.

20           18.    The method of claim 12, wherein said viewing apparatus is a CCD camera.

          19.    The method of claim 12, wherein said source of power comprises at least one motor.

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          20.    The method of claim 12, wherein said plurality of angles ranges from 0° to 90°.

          21.    The method of claim 12, wherein said positioning of said sample  
30    involves a least squares of offset data collected along said three orthogonal axes at said plurality of angles fit to an equation.

22. The method of claim 21, wherein said equation is

$$V_i = \Delta X \cos \phi_i + \Delta Y \sin \phi_i$$

5 where  $V_i$  represents the vertical offset of the centroid of the image of said sample at an angle  $\phi_i$ , and  $\Delta X$  represents the unknown offset of the centroid of the image of the sample on the X-axis and  $\Delta Y$  the represents the unknown offset of the centroid of the image of the sample on the Y-axis.

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23. The method of claim 22, wherein said equation for said third of said three orthogonal axes employs a simple average of offset data at said plurality of angles.

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24. A device for holding a crystal comprising:

- (a) a base;
- (b) an attachment element projecting from said base;
- (c) a stem projecting from said attachment element, said stem

supporting a loop for holding said crystal; and

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(e) at least one aperture in said attachment element for allowing venting of said device, said device capable of being attached to both a storage cell and a positioning device.

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25. The device of claim 24, wherein said base is cylindrical in shape.

26. The device of claim 25, wherein said base comprises a notch for locking said device to a sample rack.

27. The device of claim 24, wherein said attachment element is  
30 cylindrical in shape.

28. The device of claim 24, wherein said pin is cylindrical in shape.

29. The device of claim 24, wherein said device is attractable to a magnet.

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30. The device of claim 24, wherein said attachment element is threaded.

31. An apparatus for retrieving a crystal holder from a storage cell  
10 comprising:

(a) a rotatable element capable of retrieving the crystal holder from the storage cell;

(b) a means for rotating a rotatable element in a given direction of  
15 rotation when said rotating means is in a locked mode;

(c) a means for providing a controlled amount of torque when said rotating means is slipping relative to said rotatable element; and

(d) a means for activating said rotating means and said torque controlling means.

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32. An apparatus for retrieving a crystal holder from a storage cell, comprising:

(a) a clutch having a cylindrical housing, said housing comprising a bore surrounded by a wall;

(b) a cylindrical plunger capable of moving axially within said bore of  
25 said housing;

(c) said plunger having at least one elongated groove on the exterior periphery thereof, said groove capable of receiving a locking pin;

(d) said housing having at least one aperture extending through said  
30 wall thereof;

(e) at least one spring pin retained in said aperture, said pin capable of engaging said elongated groove when said plunger is disposed in a first position in said housing, said spring pin capable of disengaging said elongated groove when said plunger is disposed in a second position in said housing;

5 (f) a means in said housing for resiliently biasing said plunger toward said first position in said housing;

(g) an annular ring in contact with said interior wall of said housing, said ring providing friction between an output flange and a friction plate; and

(h) a shaft attached to said plunger, said shaft capable of transmitting  
10 torque to said friction plate, said shaft further capable of moving axially with respect to the friction plate.

33. The apparatus of claim 32, further including an input flange.

15 34. The apparatus of claim 33, further including means for providing axial compliance of said output flange relative to said input flange.

35. A device for holding a plurality of samples, said device comprising a plurality of storage cells, each of said storage cells having a base and an  
20 opening, the area of said opening greater than the area of said base, at least one side wall circumscribing said base and said opening, said base being of sufficient area to allow placement of a sample holder, said opening being of sufficient area to allow ingress of a tool for retrieving said sample holder, said base having attached thereto a means for locking said sample holder to said device.

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36. The device of claim 35, wherein said means for locking said sample holder to said device is a locking pin.

37. The device of claim 35, wherein said base of said device is  
30 ferromagnetic.

38. A device suitable for moving a crystal holder from a storage cell to a positioning device, said moving device comprising an elongated element having a first end and a second end, said first end capable of being linked to a robot, said second end capable of being coupled to said crystal holder, said  
5 device capable of maintaining a crystal in said crystal holder at a temperature no higher than about 160 ° K when said second end is couple to said crystal holder.

39. The device of claim 38, further including a vent to allow air to escape from said device.  
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40. A device suitable for moving a crystal holder from a storage cell to a positioning device, said moving device comprising an elongated element having a first end and a second end, said first end capable of being linked to a robot, said second end capable of being coupled to said crystal holder, said  
15 device capable of shielding said crystal holder from ambient air when said second end is couple to said crystal holder.

41. The device of claim 40, further including a vent to allow air to escape from said device.  
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